FINITE-ELEMENT Z-MATRIX CALCULATION OF ELECTRON-N_2 COLLISIONS

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The finite element Z-matrix method has been applied in a multichannel study of e-N_2 collisions for electron energies from threshold to 30 eV. General agreement is obtained comparing with existing experimental and theoretical data. Some discrepancies are also found.

The finite element Z-matrix (FEMZMX) method is a newly developed method for treating electron-molecule collisions.[1] It is based on a Kohn variational principle for finite-range scattering functionals and employs a mixed basis of Gaussians and finite elements to describe the continuum electron. The associated computer code is capable of handling target of arbitrary symmetry and sophisticated target wave functions.

We have applied the FEMZMX method to study e-N_2 collisions. Due to the role of N_2 in a variety of natural phenonmena and applied problems, e-N_2 collisions have been well studied both experimentally and theoretically. Nevertheless, experimental data so far are incomplete, covering only selected transitions at a few energies. On the theoretical side, The R-matrix calculation of Gillan et al.[2] coupling the ground and seven optically forbidden states is the most recent study on this system. While their calculation agrees with experiment in some transitions, outstanding discrepancies appear in others.

The present calculations uses the same eight states, $X^1\Sigma_g^+$, $A^3\Sigma_u^+$, $B^3\Pi_g$, $W^3\Delta_u$, $B'\,^3\Sigma_u^-$, $a'\,^1\Sigma_u^-$, $a^1\Pi_g$, and $W^1\Delta_u$ states. The target states are represented using averaged CASSCF functions and the cc-PVTZ Gaussian basis of Dunning et al. is used in the calculation. In the first region of the Z-matrix calculation, a 20 element basis with element boundaries at 0, 0.1, 0.2, 0.4, 0.6, 0.8, 1.0, 1.25, 1.5, 1.75, 2.0, 2.50, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0 is used to represent the continuum electron, with spherical harmonics expansion limited to $l \leq 6, |m| \leq 3$. This representation is supplemented by a set of Gaussian functions. In the outer region, 20 elements with Δr =1 is used in each sector. In total 200 sectors are employed. Calculations have been carried out at R_o of the ground state as well as selected R values.

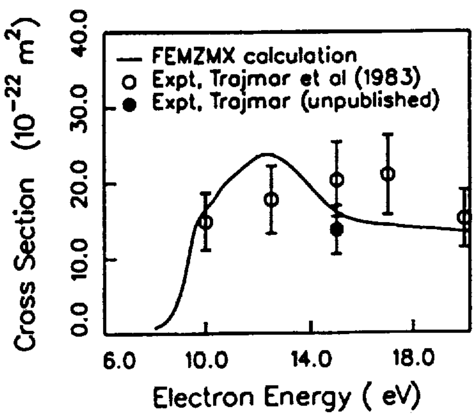

Figure 1. N_2 $X^1\Sigma_g^+ \rightarrow A^3\Sigma_u^+$ excitation cross sections by electron impact. 8 coupled state FEMZMX calculation at R_o of the ground state.

Figure 1 presents the $X^1\Sigma_g^+ \rightarrow A^3\Sigma_u^+$ electron impact excitation cross section. Comparison is made with the experiment of Trajmar et al.[4] and a new data point from Trajmar's group.[5] It is seen that there are general agreement with experiment, but the detailed energy dependence is different. Cross sections for other transitions will be presented at the conference.

<u>References</u>

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